Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 AUG 2006 HIGHEST RN 897851-29-5
DICTIONARY FILE UPDATES: 1 AUG 2006 HIGHEST RN 897851-29-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

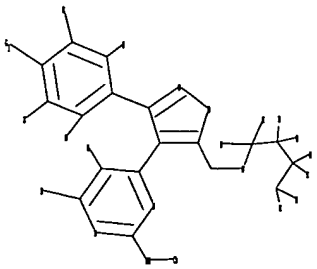
TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

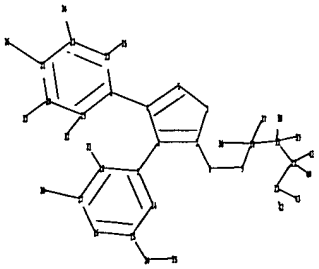
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10657811isoxazole.str





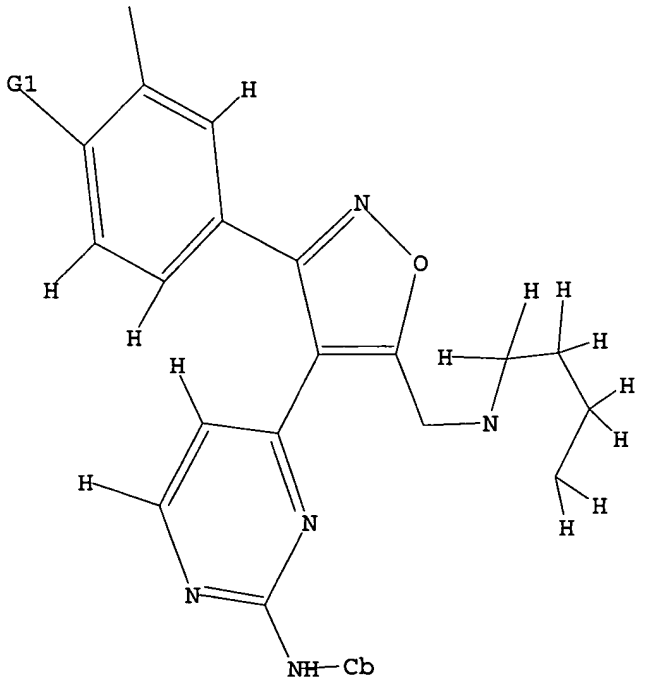
chain nodes :
8 24 25 26 30 31 32 33 34 35 36 37 38 39 40 41 42 43
ring nodes :
1 2 3 4 5 6 7 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
chain bonds :
2-8 3-7 4-6 8-9 10-36 10-37 11-12 11-38 11-39 12-40 12-41 13-42 13-43
15-24 17-30 18-31 19-32 20-33 21-26 22-34 23-35 24-25
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-19 6-23 7-14 7-18 9-10 10-11 12-13 14-15 15-16
16-17 17-18 19-20 20-21 21-22 22-23
exact/norm bonds :
4-5 8-9 9-10 10-11 12-13 15-24 21-26
exact bonds :
1-2 1-5 2-3 2-8 3-4 3-7 4-6 10-36 10-37 11-12 11-38 11-39 12-40 12-41
13-42 13-43 17-30 18-31 19-32 20-33 22-34 23-35 24-25
normalized bonds :
6-19 6-23 7-14 7-18 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
isolated ring systems :
containing 1 : 6 : 7 : 9 : 10 : 11 : 12 : 13 :

G1:H,Cl,Br,F,I

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:Atom 26:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS
40:CLASS 41:CLASS 42:CLASS 43:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Cl,Br,F,I

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss sam
SAMPLE SEARCH INITIATED 15:37:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        3 TO ITERATE

100.0% PROCESSED        3 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            3 TO      163
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 15:37:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       52 TO ITERATE

100.0% PROCESSED       52 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

L3            0 SEA SSS FUL L1

=> log hold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   166.94     167.15

 SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 15:37:18 ON 03 AUG 2006

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSPTAEXO1623

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 15:39:04 ON 03 AUG 2006
FILE 'REGISTRY' ENTERED AT 15:39:04 ON 03 AUG 2006
COPYRIGHT (C) 2006 American Chemical Society (ACS)

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   166.94     167.15

=>
Uploading C:\Program Files\Stnexp\Queries\10657811isoxazole2.str
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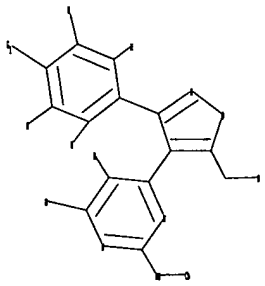
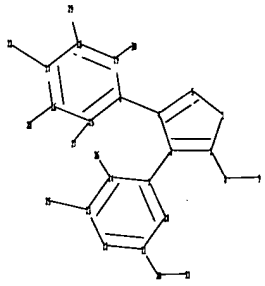




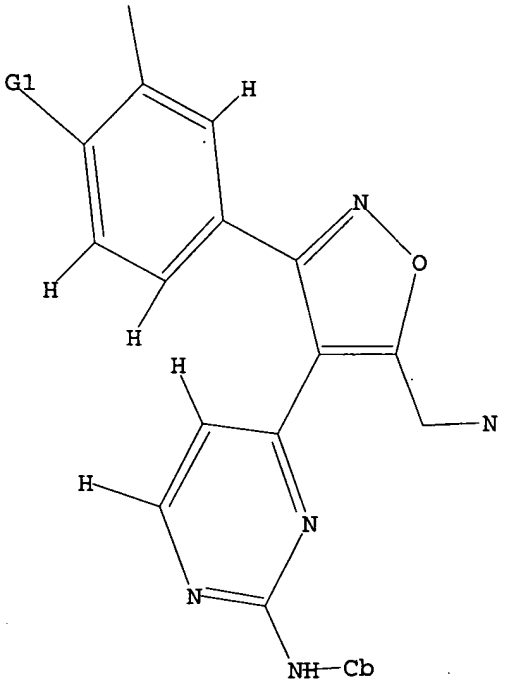
chain nodes :
8 20 21 22 25 26 27 28 29 30
ring nodes :
1 2 3 4 5 6 7 9 10 11 12 13 14 15 16 17 18 19
chain bonds :
2-8 3-7 4-6 8-9 11-20 13-25 14-26 15-27 16-28 17-22 18-29 19-30 20-21
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-15 6-19 7-10 7-14 10-11 11-12 12-13 13-14 15-16
16-17 17-18 18-19
exact/norm bonds :
4-5 8-9 11-20 17-22
exact bonds :
1-2 1-5 2-3 2-8 3-4 3-7 4-6 13-25 14-26 15-27 16-28 18-29 19-30 20-21
normalized bonds :
6-15 6-19 7-10 7-14 10-11 11-12 12-13 13-14 15-16 16-17 17-18 18-19
isolated ring systems :
containing 1 : 6 : 7 : 9 :

G1:H,Cl,Br,F,I

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:Atom 22:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR



G1 H,Cl,Br,F,I

Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 15:39:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3 TO 163
PROJECTED ANSWERS: 3 TO 163

L5 3 SEA SSS SAM L4

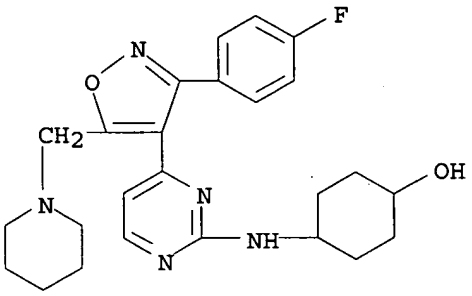
=> scan l5
ENTER FIELD CODE (BI):bi
E1 11 L4R/BI
E2 4 L4S2/BI

```
E3         1137 --> L5/BI
E4            3     L5'/BI
E5            2     L5'HER13/BI
E6           20     L5.1/BI
E7            1     L5.2/BI
E8            1     L5.3/BI
E9            3     L5.4/BI
E10          26     L5.5/BI
E11           2     L5A/BI
E12          45     L50/BI

=> d l5 scan

L5    3 ANSWERS   REGISTRY  COPYRIGHT 2006 ACS on STN
IN    Cyclohexanol, 4-[[4-[3-(4-fluorophenyl)-5-(1-piperidinylmethyl)-4-
      isoxazolyl]-2-pyrimidinyl]amino]-, mono(trifluoroacetate) (salt) (9CI)
MF    C25 H30 F N5 O2 . C2 H F3 O2

      CM   1
```

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      CM   2
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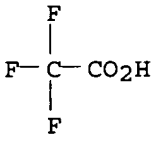
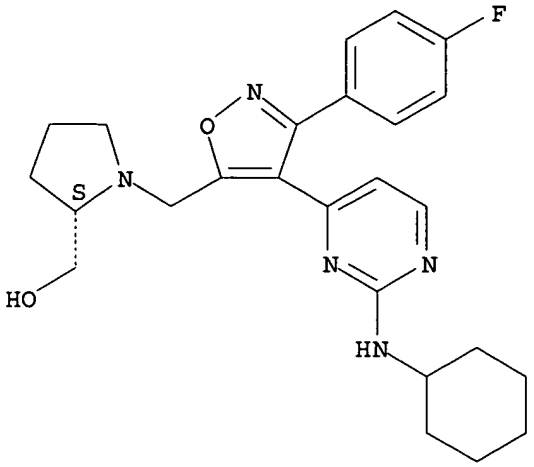



```
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

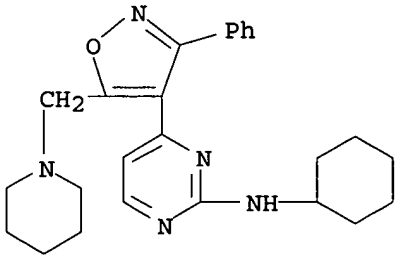
L5    3 ANSWERS   REGISTRY  COPYRIGHT 2006 ACS on STN
IN    2-Pyrrolidinemethanol, 1-[[4-[2-(cyclohexylamino)-4-pyrimidinyl]-3-(4-
      fluorophenyl)-5-isoxazolyl]methyl]-, (2S)- (9CI)
MF    C25 H30 F N5 O2

Absolute stereochemistry.
```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Pyrimidinamine, N-cyclohexyl-4-[3-phenyl-5-(1-piperidinylmethyl)-4-isoxazolyl]- (9CI)
MF C25 H31 N5 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

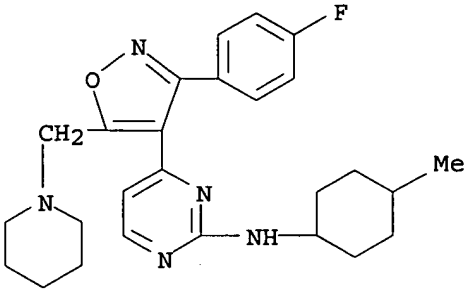
=> s l4 sss full
FULL SEARCH INITIATED 15:40:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS 29 ANSWERS
SEARCH TIME: 00.00.01

L6 29 SEA SSS FUL L4

=> d l6 scan

L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Pyrimidinamine, 4-[3-(4-fluorophenyl)-5-(1-piperidinylmethyl)-4-isoxazolyl]-N-(4-methylcyclohexyl)- (9CI)
MF C26 H32 F N5 O

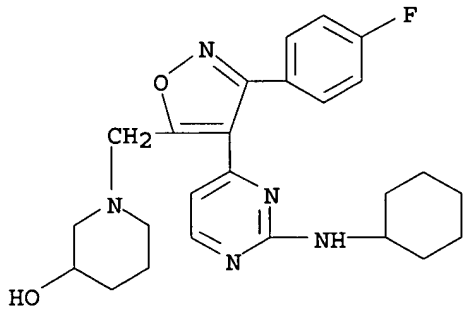


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

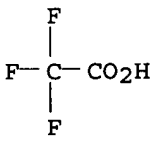
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 3-Piperidinol, 1-[[4-[2-(cyclohexylamino)-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]-, mono(trifluoroacetate) (salt) (9CI)
MF C25 H30 F N5 O2 . C2 H F3 O2

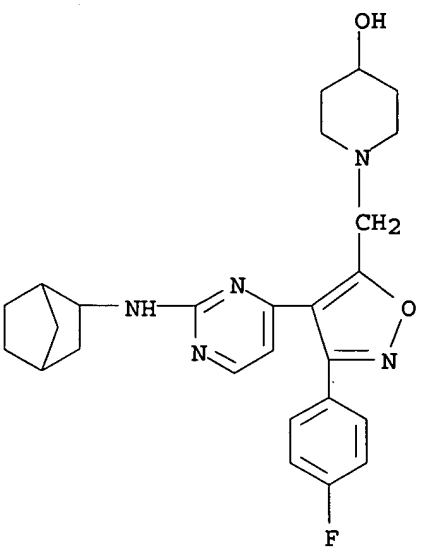
CM 1



CM 2



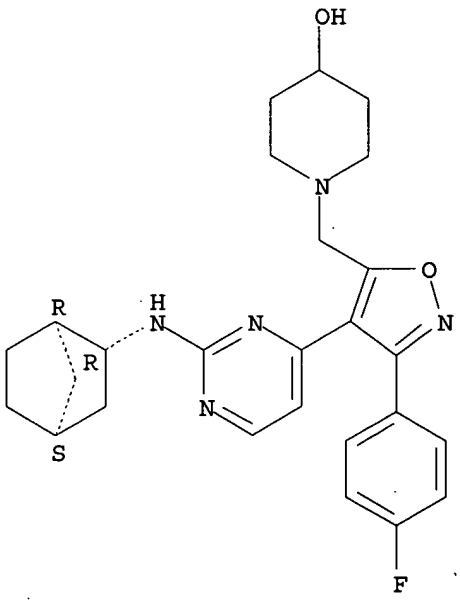
L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 4-Piperidinol, 1-[[4-[2-(bicyclo[2.2.1]hept-2-ylamino)-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]-, dihydrochloride (9CI)
MF C26 H30 F N5 O2 . 2 Cl H



● 2 HCl

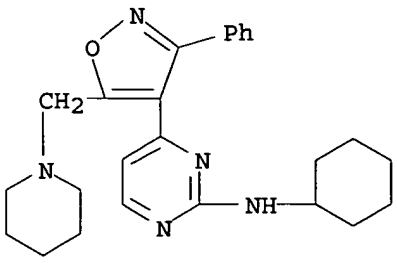
L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 4-Piperidinol, 1-[[4-[2-[(1R,2R,4S)-bicyclo[2.2.1]hept-2-ylamino]-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]- (9CI)
MF C26 H30 F N5 O2
CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Pyrimidinamine, N-cyclohexyl-4-[3-phenyl-5-(1-piperidinylmethyl)-4-isoxazolyl]- (9CI)
MF C25 H31 N5 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> sel l6
E1 THROUGH E29 ASSIGNED

=> index bioscience paents
FILE 'DRUGMONOG' ACCESS NOT AUTHORIZED
'PAENTS' IS NOT A VALID FILE NAME
ENTER A FILE NAME OR (IGNORE):patents
FILE 'ENCOMPPAT2' ACCESS NOT AUTHORIZED

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	344.77	344.98

INDEX 'ADISCTI, ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, ANTE, AQUALINE, AQUASCI, BIOENG, BIOSIS, BIOTECHABS, BIOTECHDS, BIOTECHNO, CABA, CAPLUS, CEABA-VTB, CIN, CONFSCI, CROPB, CROPU, DDFB, DDFU, DGENE, DISSABS, DRUGB, DRUGMONOG2, DRUGU, EMBAL, EMBASE, ...' ENTERED AT 15:41:41 ON 03 AUG 2006

92 FILES IN THE FILE LIST IN STNINDEX

Enter SET DETAIL ON to see search term postings or to view
search error messages that display as 0* with SET DETAIL OFF.

=> s E1-E29
          2   FILE CAPLUS
  30 FILES SEARCHED...
  64 FILES SEARCHED...
  68 FILES SEARCHED...
  87 FILES SEARCHED...

   1 FILES HAVE ONE OR MORE ANSWERS,   92 FILES SEARCHED IN STNINDEX

L7   QUE (326817-96-3/BI OR 673451-34-8/BI OR 673451-35-9/BI OR 673451-36-0/BI
         OR 673451-37-1/BI OR 673451-38-2/BI OR 673451-39-3/BI OR 673451-40-6/B
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         451-60-0/BI OR 673451-61-1/BI)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.22	346.20

FILE 'CAPLUS' ENTERED AT 15:43:08 ON 03 AUG 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 3 Aug 2006 VOL 145 ISS 6
FILE LAST UPDATED: 1 Aug 2006 (20060801/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l6
L8 2 L6

=> d l8 1-2 ti abs bib

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
TI Preparation of isoxazoles and their use in the treatment of ischemic diseases
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H or halo; R2 = (un)substituted cycloalkyl; R3 for each occurrence independently = halo, alkyl, hydroxyalkyl, alkoxyalkyl, etc.; m = 0-2; n = 0-2] and their pharmaceutically acceptable salts are prepared and disclosed as useful for the treatment of neurol., neurodegenerative, ischemic and inflammatory disorders. Thus, e.g., II was prepared in 95% yield via substitution of 3-(4-fluorophenyl)-4-(3-methylsulfonylpyrimidin-4-yl)-5-(4-hydroxypiperidin-1-ylmethyl)isoxazole (preparation given) with cyclohexylamine. Preferred compds. of the invention demonstrated a protection value of ≥ 50% in in vitro ischemia assay. Addnl., compds. were evaluated in in vitro CNS inflammation assays and preferred compds. possessed IC50 values of 300 nM or less. Accordingly, the invention also provides pharmaceutically acceptable compns. comprising the compds. of the invention and methods of utilizing those compds. and compns. in the treatment of neurol., neurodegenerative, ischemic and inflammatory disorders.
AN 2004:220330 CAPLUS
DN 140:270843
TI Preparation of isoxazoles and their use in the treatment of ischemic diseases
IN Ledeboer, Mark; Ledford, Brian; Maltais, Francois
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI WO 2004022555 A1 20040318 WO 2003-US27903 20030908
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2003270350 A1 20040329 AU 2003-270350 20030908
US 2004132755 A1 20040708 US 2003-657811 20030908
EP 1546141 A1 20050629 EP 2003-752038 20030908
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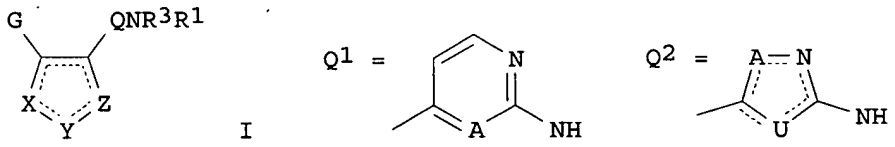
JP 2006502168 T2 20060119 JP 2004-534669 20030908
PRAI US 2002-408813P P 20020906
WO 2003-US27903 W 20030908
OS MARPAT 140:270843
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
TI Preparation of as isoxazolylpyrimidines and related compounds as inhibitors of c-JUN N-terminal kinases and other protein kinases.
GI



AB Title compds. [I; XYZ = NOCR2, ON:CR2, N:NNR3, OC(R2):CR2, NN(R3)CR2; R1 = H, CONH2, TnR, TnAr2; R = (substituted) aliphatyl; n = 0, 1; T = CO, CO2, CONH, SO2, SO2NH, COCH2, CH2; R2 = H, R, CH2OR, CH2OH, CHO, CH2SR, CH2SO2R, CH2NH2, CH2CN, (substituted) aryl, arylmethyl, heterocyclyl, heterocyclylmethyl, etc.; R3 = H, R, COR, CO2R, SO2R; G = R, Ar1; Ar1 = (substituted) (fused) aryl, aralkyl, heterocyclyl; Q = Q1, Q2; A = N, CR3; U = CR3, O, S, NR3; Ar2 = (substituted) (fused) aryl, heterocyclyl], were prepared Thus, 4-(5-methyl-3-phenylisoxazole-4-yl)pyrimidin-2-ylamine (preparation given) was refluxed with PhBr, tris(dibenzylideneacetone)dipalladium, BINAP, and NaOCMe3 were refluxed together for 16 h to give 36% 4-(5-methyl-3-phenylisoxazole-4-yl)pyrimidin-2-ylphenylamine. Several I inhibited KNK3 at <0.1 μM.
AN 2001:137207 CAPLUS
DN 134:178569
TI Preparation of as isoxazolylpyrimidines and related compounds as inhibitors of c-JUN N-terminal kinases and other protein kinases.
IN Green, Jeremy; Bemis, Guy; Grillot, Anne-Laure; Ledeboer, Mark; Salituro, Francis; Harrington, Edmund; Gao, Huai; Baker, Christopher; Cao, Jingrong; Hale, Michael
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001012621	A1	20010222	WO 2000-US22445	20000811

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         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
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OS   MARPAT 134:178569
RE.CNT  11    THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> d his

     (FILE 'HOME' ENTERED AT 15:36:35 ON 03 AUG 2006)

     FILE 'REGISTRY' ENTERED AT 15:36:45 ON 03 AUG 2006
L1              STRUCTURE UPLOADED
L2            0 S L1 SSS SAM
L3            0 S L1 SSS FULL
L4              STRUCTURE UPLOADED
L5            3 S L4
                SCAN L5 BI
L6           29 S L4 SSS FULL
                SEL L6

     INDEX 'ADISCTI, ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, ANTE, AQUALINE,
     AQUASCI, BIOENG, BIOSIS, BIOTECHABS, BIOTECHDS, BIOTECHNO, CABA, CAPLUS,
     CEABA-VTB, CIN, CONFSCI, CROPB, CROPU, DDFB, DDFU, DGENE, DISSABS, DRUGB,
     DRUGMONOG2, DRUGU, EMBAL, EMBASE, ...' ENTERED AT 15:41:41 ON 03 AUG 2006
                SEA E1-E29
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               2   FILE CAPLUS
L7              QUE (326817-96-3/BI OR 673451-34-8/BI OR 673451-35-9/BI OR 6734
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     FILE 'CAPLUS' ENTERED AT 15:43:08 ON 03 AUG 2006
L8            2 S L6

=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    5.94     352.14
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.50	-1.50

STN INTERNATIONAL LOGOFF AT 15:43:41 ON 03 AUG 2006